Supplementary Material (ESI) for Dalton Transactions

Supporting information

New possible mode of ligand-metal cooperation in PC(sp^3)P pincer complexes

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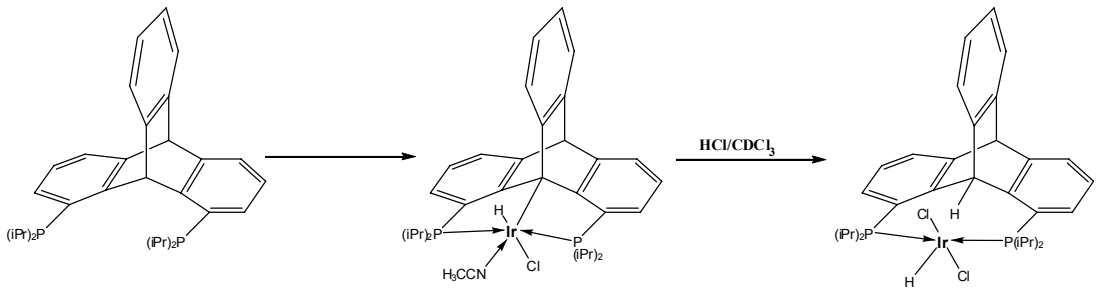
General Considerations. All manipulations were performed using standard Schlenk techniques under dry N_2 or Ar. All reagents were purchased from the usual suppliers and used without further purification**.** All reagents were weighed and handled in air. ^{1}H-, ^{13}C- and ^{31}P-NMR spectra were recorded on a Bruker 400 or 500 MHz instruments with chemical shifts reported in ppm relative to the residual deuterated solvent or the internal standard tetramethylsilane. Diffraction data were collected with a Bruker APEX CCD instrument (MoKα radiation (λ = 0.71073Å)). Crystals were mounted onto glass fibers using epoxy. Single crystal reflection data were collected on a Bruker APEX CCD X-ray diffraction system controlled by a Pentium-based PC running the SMART software package.[2] The integration of data frames and refinement of cell structure were done by the SAINT+ program package.[3] Refinement of the structure **8** on F^2 was carried out by the SHELXTL software package.[4]

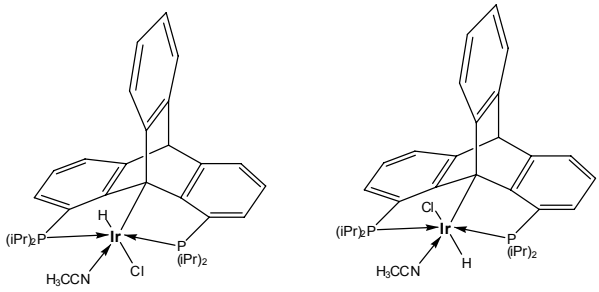
Experimental Details:



1 **3**

Synthesis of 1. 1,8-bis-(diisopropylphosphino)triptycene was prepared as was described in Grossman et al. *Organometallics*, 2006, **25**, 375-381.

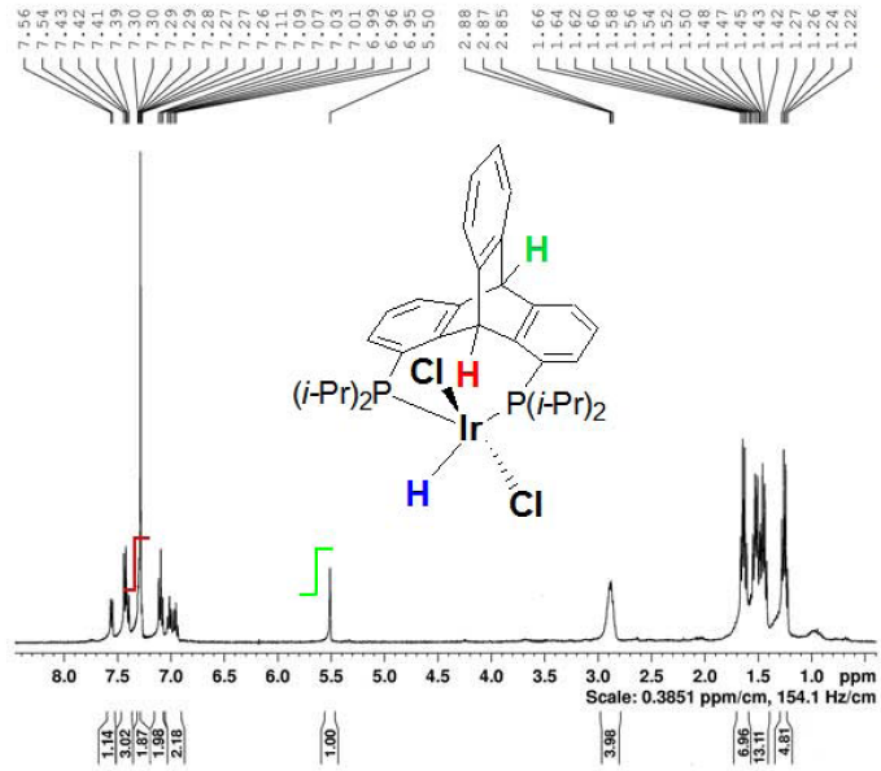
$[IrCl(COE)_2]_2$ (0.255 g, 0.28 mmol) was added to a solution of 1,8-bis-(diisopropylphosphino) triptycene (0.277 g, 0.57 mmol) in 15 ml of acetonitrile. The contents were stirred at RT for 7 hours and evaporated, affording **1** as a green solid (0.385 g, 0.5 mmol, 88% yield). The product consists of two stereoisomers (4:1). The exact structure of the compounds was determined after carbonylation of the compounds and comparing their spectral features with the previously reported carbonyl complexes (C. Azerraf et al. *Organometallics*, 2009, **28**, 6578-6584).



Major isomer. ^{1}H-NMR ($CDCl_3$), δ: 7.52 (1H, d, J = 7 Hz), 7.31 (2H, d, J = 7Hz), 7.05 (2H, d, J = 7 Hz); 6.98-7.01 (3H, m), 6.81-6.88 (2H, m), 5.32 (1H, s), 3.32 (2H, m), 1.66-1.75 (6H, m); 1.45-1.57 (12H, m), 1.12-1.22 (6H, m), -21.84 (1H, t, J = 12 Hz); ^{31}P-NMR ($CDCl_3$), δ: 37.47.

Synthesis of 3. HCl prepared *in situ* from MeOH (20 mL)/AcCl (6 mL) was bubbled through the solution of 1 (50 mg) in $CHCl_3$ (4 mL). The flask was sealed and left with stirring for 18 hours. The Solvent was evaporated affording **3** as a white powder (34 mg, 0.048 mmol, 72% yield).

^{1}H-NMR ($CDCl_3$), δ: 7.55 (1H, d, J = 4Hz), 7.39-7.43 (3H, m), 7.3 (2H, s), 7.29 (1H, s), 7.07-7.26 (2H, m), 6.95-7.03 (2H,m), 5.50 (1H, s), 2.87 (4H, m), 1.22-1.66 (24H, m), -30.96 (1H, t, J = 8 Hz); ^{31}P-NMR ($CDCl_3$), δ: 29.24 (s). Anal. Calcd. For $C_{32}H_{41}Cl_2IrP_2$: C, 51.20; H, 5.50. Found: C, 51.68; H, 5.81.



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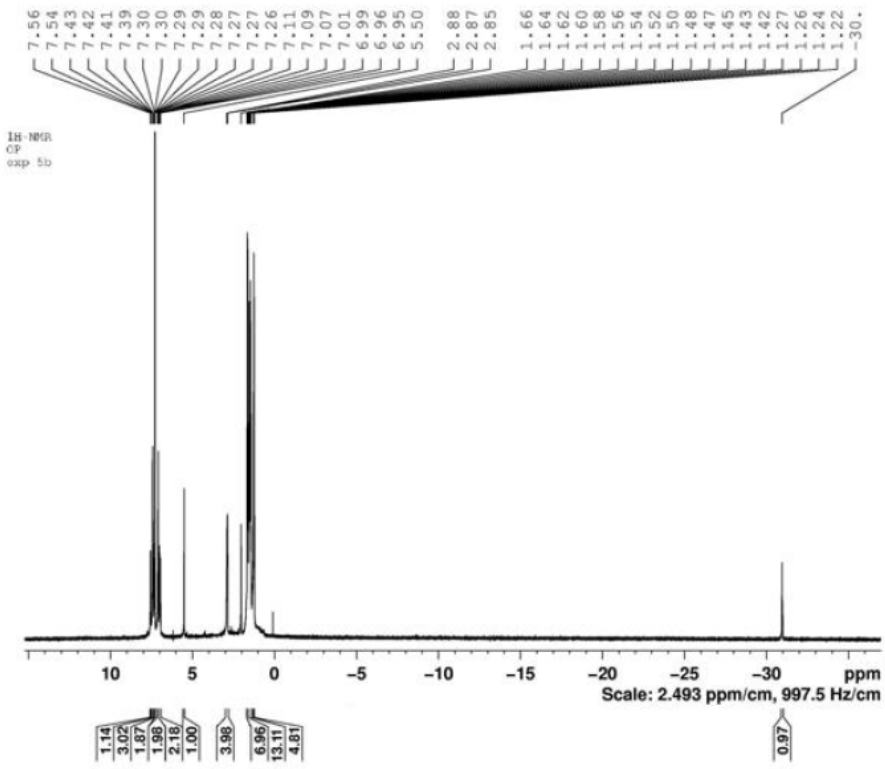

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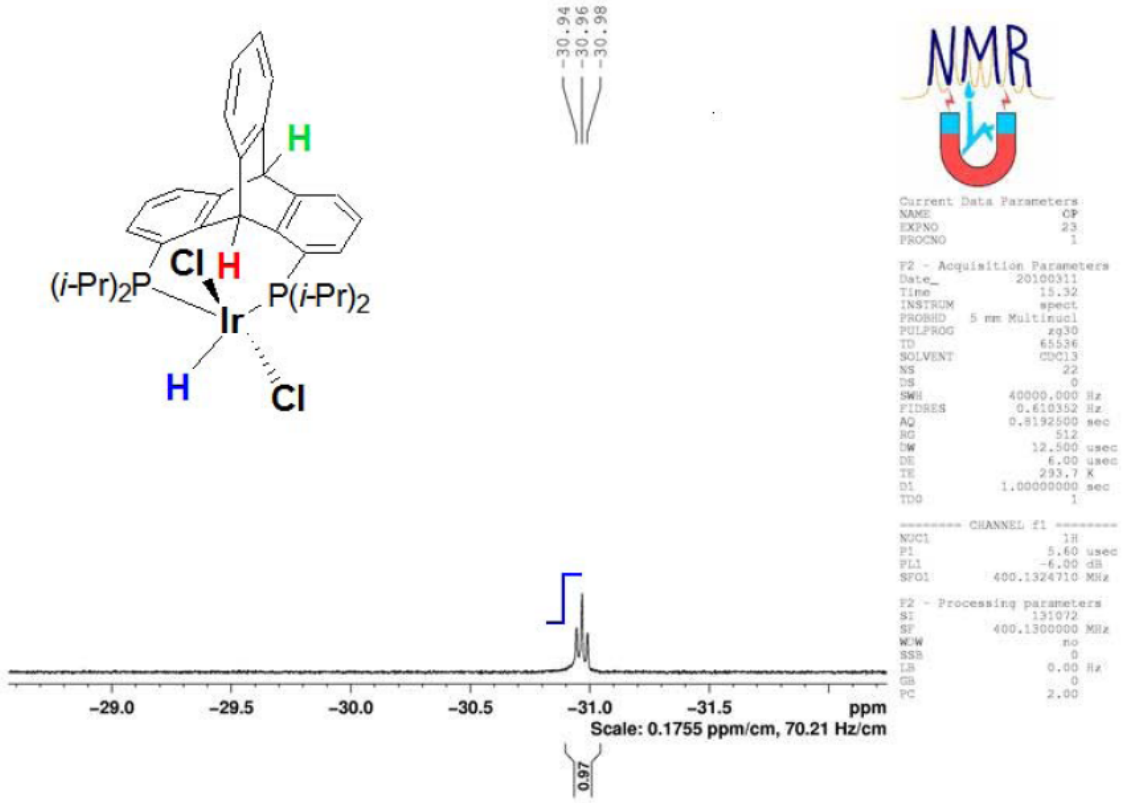
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P(i-Pr)2
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-31.5
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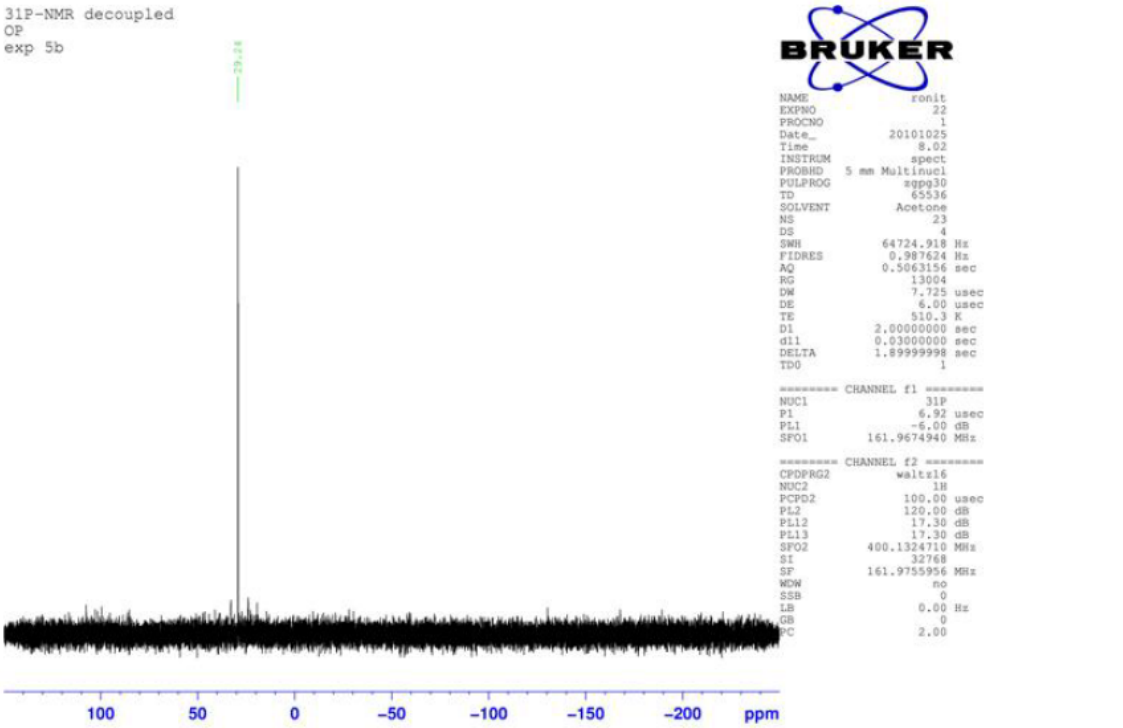
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PL13 17.30 dB
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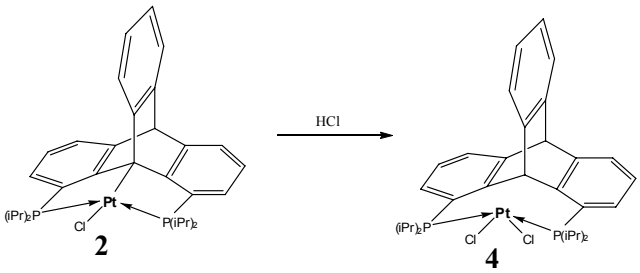
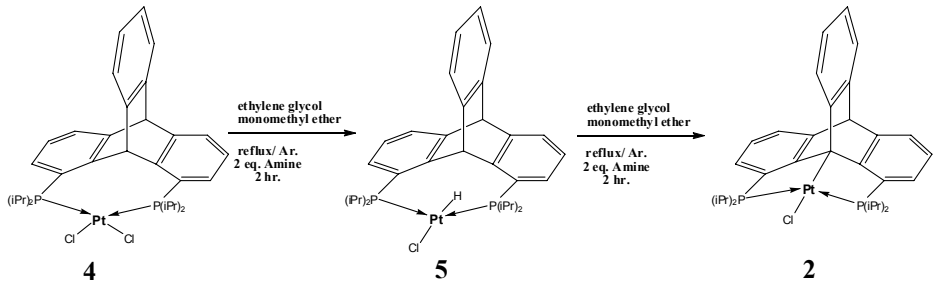
ppm



Synthesis of 5. 2 was prepared as was described previously in C. Azerraf et al. *Organometallics*, 2009, **28**, 6578-6584.

Synthesis of 4. HCl was bubbled through the solution of complex **2** (20 mg) in dry CH_2Cl_2 (1 mL) for 2 hours. The flask sealed and heated to 40 ^oC overnight. The solvent was evaporated affording the mixture of **4** (^{31}P-NMR δ: 1.93 (J_{Pt-P} = 1848 Hz); ca. 15% NMR yield) and two unidentified by-products (^{31}P-NMR δ: 42.12 and 39.41 ppm).

The spectral data of **4** was compared to the previously published (Azerraf et al. *J. Organomet. Chem.* 2007, **692**, 761).

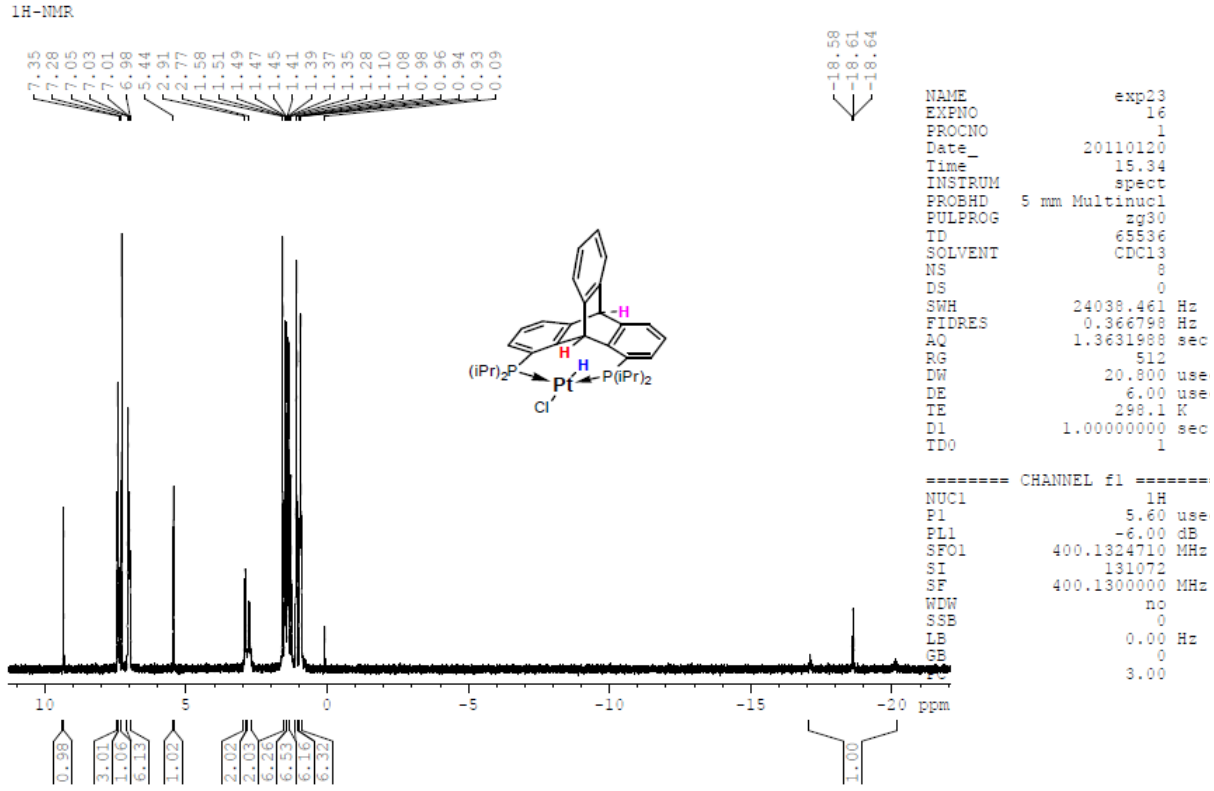


Synthesis of 5. 4 was prepared as was described previously in Azerraf et al. *J. Organomet. Chem.* 2007, **692**, 761.

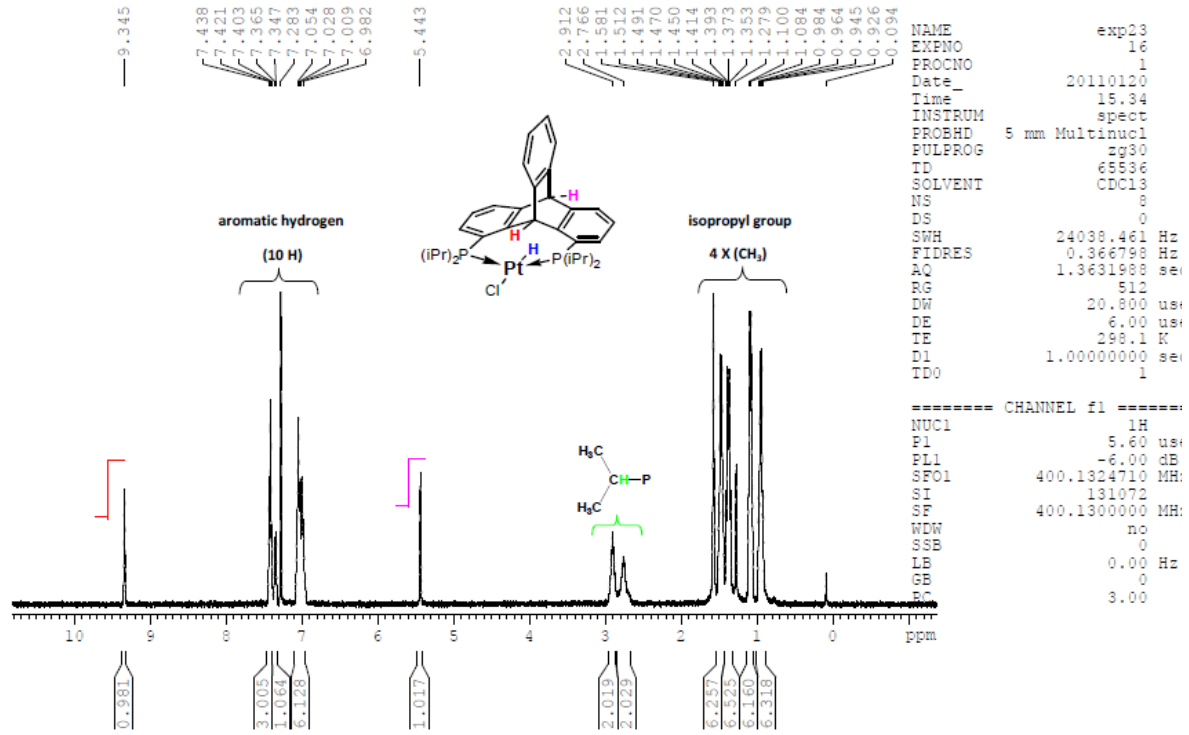
The solution of **4** (0.25 gr, 0.26 mmol) and diisopropylamine (0.1 ml, 0.52 mmol) in 10 ml of ethylene glycol monomethyl ether was refluxed for 2 hours under Argon flow. The solvent was evaporated and the product **5** was rinsed with methanol and dried affording 0.15 gr (77%) of white solid.

If the reaction continued for additional 12 hours formation of **2** is observed. The spectral data of **2** is identical to the previously published.

5: ^{1}H-NMR ($CDCl_3$), δ: 9.35 (t, 3H, J=7 Hz), 7.42 (t, 3H, J = 7 Hz), 7.35 (d, 1H, J = 7 Hz), 7.01 (m, 6H), 5.44 (s, 1H), 2.91 (m, 2H), 2.76 (m, 2H), 1.50 (q, 6H, J = 8 Hz), 1.37 (q, 6H, J = 8 Hz), 1.09 (q, 6H, J = 7 Hz), 0.96 (q, 6H, J = 8 Hz), -18.61 (t, 1H, $J_{P\text{-}H}$ = 13 Hz). ^{31}P-NMR ($CDCl_3$), δ: 43.36 (t, J = 1498 Hz). Anal. Calcd. For $C_{32}H_{41}ClP_2Pt$: C, 53.52; H, 5.75. Found: C, 53.29; H, 6.03.



1H-NMR

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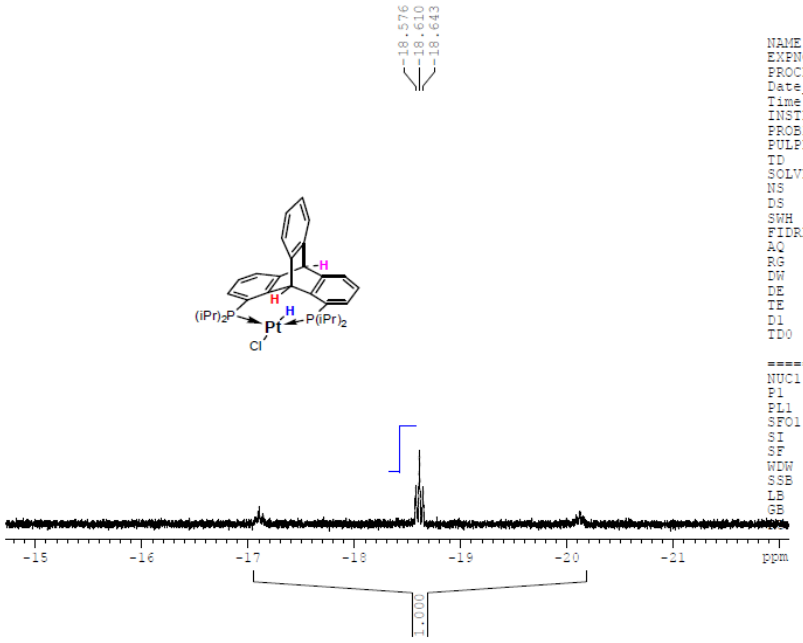
1H-NMR

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PROCNO                  1
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Time                15.34
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PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                    512
DW                20.800 usec
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TE                298.1 K
D1          1.00000000 sec
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======== CHANNEL f1 =======
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PL1                -6.00 dB
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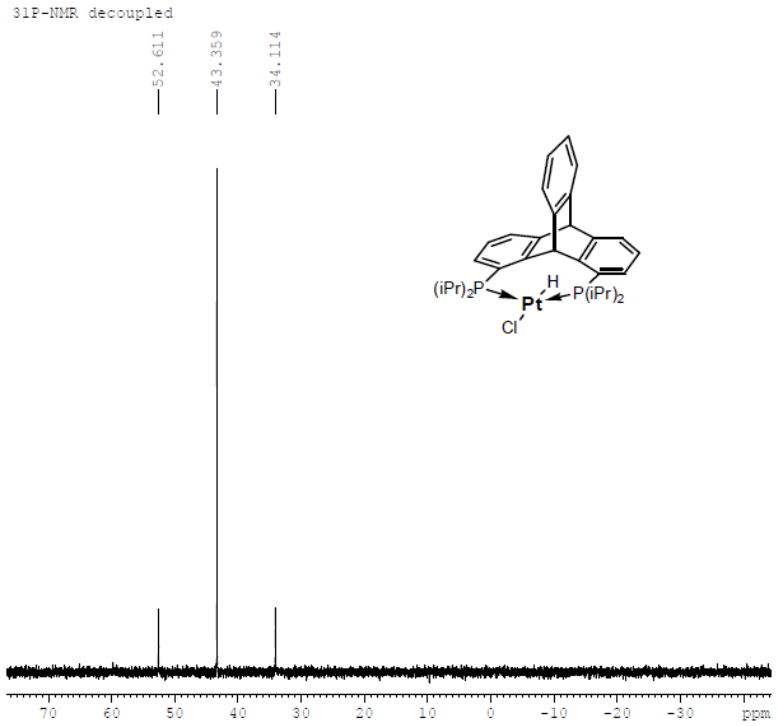


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FIDRES           0.987624 Hz
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RG                  9195.2
DW                   7.725 usec
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TE                  298.1 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                     1

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WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   2.00
```

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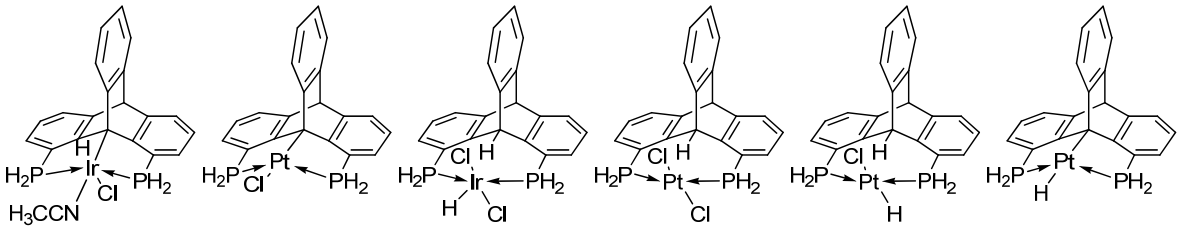
Theoretical Method:

All geometries were calculated with the B97D GGA functional (intrinsically includes a dispersion correction), at the Def2-SV(P) basis set in gas phase. Gibbs correction terms were calculated at the same level, at room temperature and standard 1M concentration (equivalent to 24.45 ATM). Single point energies were computed with the PBE0 hybrid functional, with the Def2-TZVPP basis set in the default chloroform continuum solvent model. To this energy the D3 dispersion correction energy was added.

In summary, the theoretical method is PBE0+D3/Def2-TZVPP(CHCl3)//B97D/Def2-SV(P), plus Gibbs energy correction.

To avoid conformation artifacts and to focus on the interaction of the ligands with the metal center, the phosphines were simplified by changing the *i*Pr groups to hydrogens.

Theoretical reaction energies:



1 **2** **3** **4** **5** **6**

Reaction	ΔE_{rx} (kcal/mol)	ΔG_{rx} (kcal/mol)[a]
1 + HCl → **3** + MeCN	-1.0	0.5
2 + HCl → **4**	-16.7	-4.3
2 + H_2 → **5**	-15.0	-2.9
6 + HCl → **5**	-32.6	-19.8

[a] $\Delta G_{rx} = \Delta E_{rx}$ + Gibbs energy corection terms

Supplementary Material (ESI) for Dalton Transactions

Complex 1

46

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Complex 2

39

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Complex 3

42

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H -1.430654 -3.109217 1.226401
H -2.252106 -3.119943 -0.806286
C 1.069425 1.244453 -0.532141
C 3.164312 0.000017 -0.908976
H -0.006879 -0.000191 0.977853
Cl -1.969438 0.000852 -2.167873
H 4.120417 0.000085 -1.460530
H -3.516199 -0.000150 0.213649

Complex 4

41

Pt 2.121381 -0.000057 0.317505
Cl 1.908568 -0.000437 2.712548
P 1.448328 -2.204709 0.241798
P 1.448395 2.204568 0.242416
C -1.131378 -0.000074 0.475684
C -0.185409 -2.239040 -0.617270
C -0.422651 -3.266152 -1.564748
H 0.324468 -4.060310 -1.705550
C -1.586606 -3.275105 -2.346279
H -1.745166 -4.081472 -3.076476
C -2.532933 -2.240697 -2.216585
H -3.433087 -2.223086 -2.847997
C -2.308259 -1.223368 -1.284763
C -1.152747 1.221217 -0.464483
C -0.185378 2.239218 -0.616575
C -0.422616 3.266648 -1.563710
H 0.324519 4.060834 -1.704268
C -1.586580 3.275875 -2.345222
H -1.745139 4.082485 -3.075152
C -2.532914 2.241429 -2.215864
H -3.433071 2.224034 -2.847278
C -2.308243 1.223792 -1.284380
C -2.453261 -0.000189 1.243932
C -2.579652 -0.000418 2.636884
H -1.679364 -0.000530 3.268762
C -3.872600 -0.000501 3.201020
H -3.991418 -0.000681 4.294404
C -5.010369 -0.000354 2.373653
H -6.013837 -0.000420 2.824089
C -4.875502 -0.000123 0.968854
H -5.764523 -0.000012 0.320819
C -3.591837 -0.000043 0.413275
H 1.228469 -2.813863 1.512185
H 2.129596 -3.253478 -0.443698
H 1.228688 2.813607 1.512886
H 2.129803 3.253289 -0.443003
C -1.152760 -1.221066 -0.464871
C -3.212725 0.000183 -1.068698
H -0.295229 -0.000185 1.182622
Cl 2.475636 0.000360 -2.043081
H -4.088248 0.000295 -1.741002

Complex 5

41

Pt 2.296042 -0.000042 -0.041332
Cl 2.202513 0.000206 2.446039
P 1.611218 -2.185214 -0.083678
P 1.611537 2.184923 -0.084040
C -0.928882 -0.000030 0.424617
C -0.109547 -2.233934 -0.764050
C -0.454554 -3.269402 -1.669025
H 0.270300 -4.067951 -1.884225
C -1.700963 -3.283686 -2.312367
H -1.943057 -4.097173 -3.011314
C -2.627658 -2.248088 -2.083473
H -3.594657 -2.235955 -2.607257
C -2.299159 -1.224589 -1.189708
C -1.057315 1.219121 -0.506607
C -0.109446 2.233911 -0.763946
C -0.454481 3.269510 -1.668765
H 0.270421 4.068017 -1.883964
C -1.700920 3.283927 -2.312038
H -1.943031 4.097528 -3.010848
C -2.627588 2.248268 -2.083308
H -3.594598 2.236207 -2.607075
C -2.299074 1.224654 -1.189687
C -2.154674 -0.000059 1.338143
C -2.119035 -0.000113 2.736614
H -1.150765 -0.000152 3.258408
C -3.339530 -0.000054 3.444001
H -3.332820 -0.000085 4.543851
C -4.564745 0.000049 2.752281
H -5.510069 0.000073 3.314730
C -4.592373 0.000115 1.341286
H -5.550287 0.000179 0.800078
C -3.380587 0.000070 0.642495
H 1.516628 -2.797239 1.201400
H 2.198123 -3.256694 -0.824685
H 1.517701 2.798309 1.200459
H 2.198790 3.255352 -0.826303
C -1.057356 -1.219087 -0.506723
C -3.173331 0.000061 -0.873883
H -0.017088 -0.000049 1.032042
H 2.416242 -0.000161 -1.631231
H -4.119809 0.000100 -1.442217

Complex 6

39

H -4.608792 -0.000024 1.743604
Pt 1.940478 -0.000003 0.274291
C -3.120651 -0.000011 3.345136
H 3.588284 -0.000012 0.354347
H -1.436627 -0.000006 4.718892
P 1.727936 -2.222856 -0.187235
P 1.727942 2.222855 -0.187233
C -1.752279 -0.000005 3.664867
C -0.265568 0.000003 0.071431
C -0.503167 -3.492266 -1.587456
H 0.296455 0.000011 2.869550
H 0.110168 -4.386735 -1.772577
H -3.872824 -0.000017 4.147976
C -1.842733 -3.460074 -2.008640
H -2.268183 -4.326903 -2.535235
C -2.658550 -2.337656 -1.734999
H -3.719438 -2.342225 -2.027119
C -2.113866 -1.236752 -1.065787
C -0.748153 1.235245 -0.698791
C 0.044739 2.371103 -0.923192
C -0.503161 3.492275 -1.587444
H 0.110176 4.386743 -1.772565
C -1.842729 3.460089 -2.008622
H -2.268177 4.326921 -2.535216
C -2.658550 2.337676 -1.734976
H -3.719439 2.342248 -2.027096
C -2.113868 1.236768 -1.065770
C -1.188254 0.000008 1.303582
C -0.780036 0.000007 2.640917
C -3.537303 -0.000019 1.995440
C -2.573767 -0.000010 0.982913
H 1.785639 3.274495 0.784562
H 2.607866 -2.798411 -1.151804
H 2.607869 2.798435 -1.151791
H 1.785642 -3.274513 0.784541
C 0.044732 -2.371100 -0.923193
C -2.849773 0.000003 -0.537942
H -3.927484 0.000004 -0.779877
C -0.748157 -1.235241 -0.69